JÜLICH
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Parallel I/O on JUQUEEN

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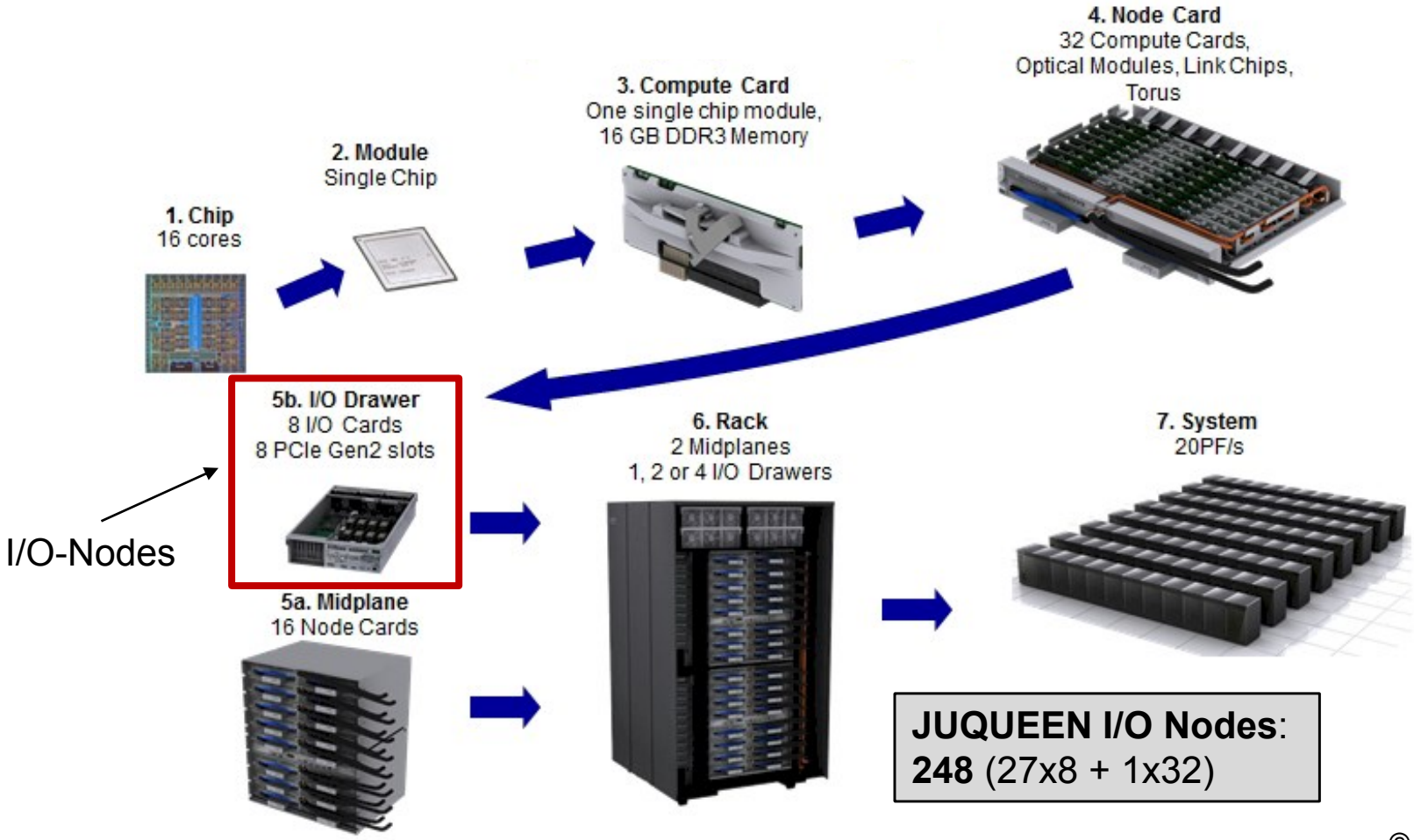
Sebastian Lührs, Kay Thust
s.luehrs@fz-juelich.de, k.thust@fz-juelich.de
Jülich Supercomputing Centre

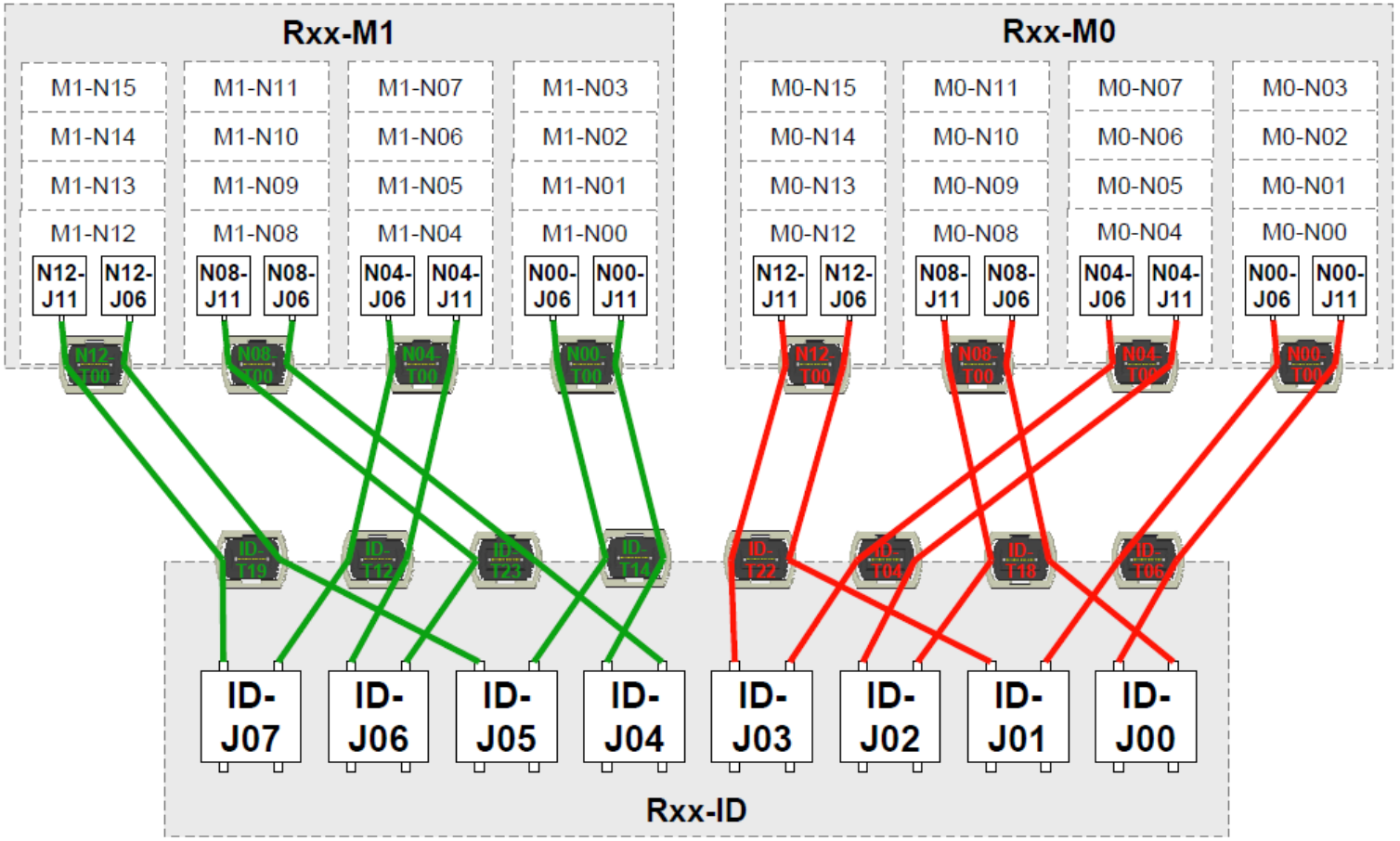
Overview

- Blue Gene/Q I/O Hardware
  - Overview, Cabling, I/O Services
- GPFS architecture and data path
- Pitfalls
- The Parallel I/O Software Stack
- Darshan
  - Overview, Usage, Interpretation
- SIONlib
- Parallel HDF5
- I/O Hints

Blue Gene/Q Packaging Hierarchy

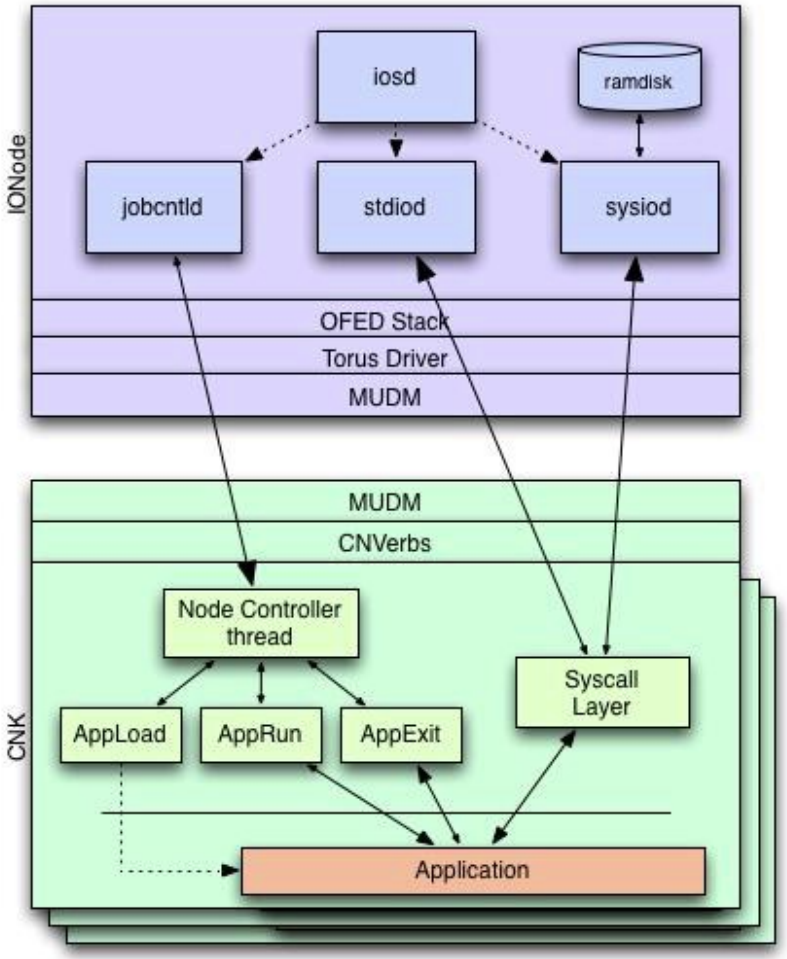


Blue Gene/Q: I/O-node cabling (8 ION/Rack)

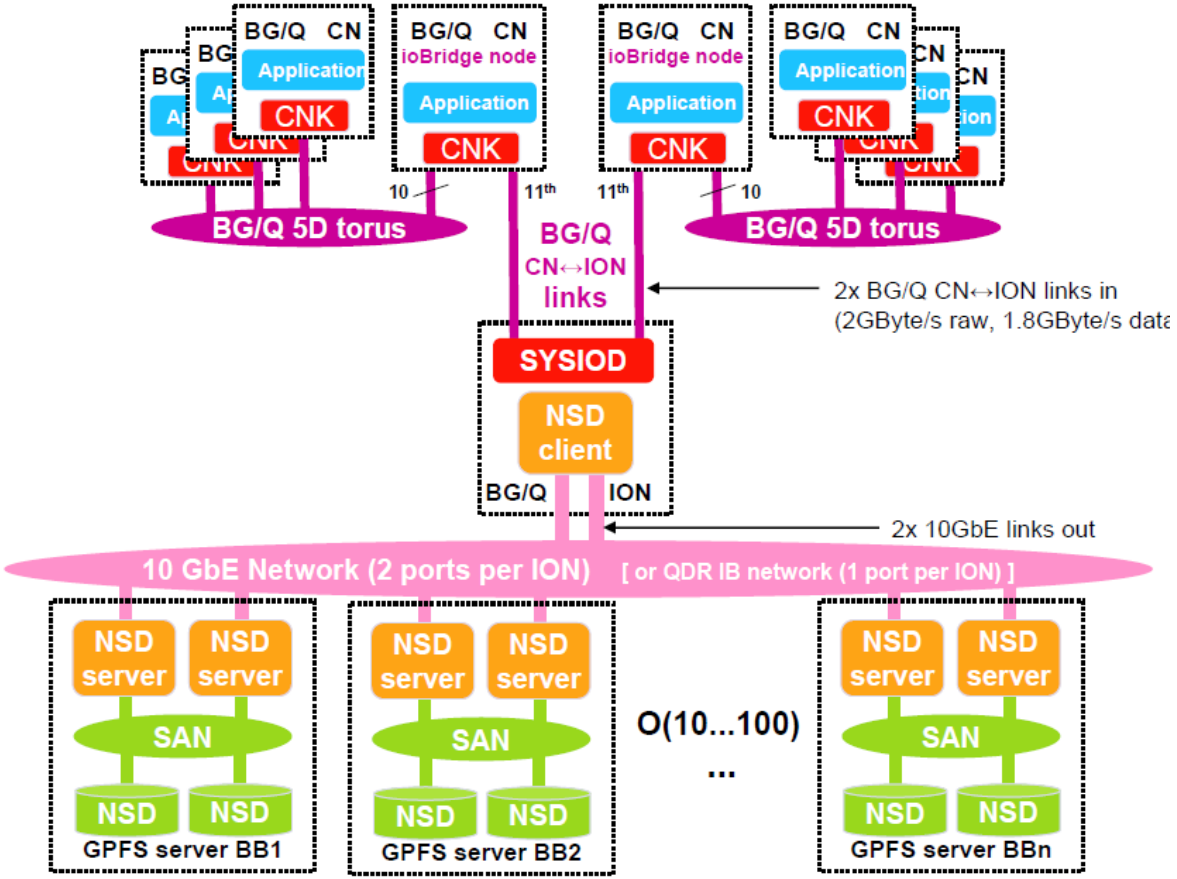


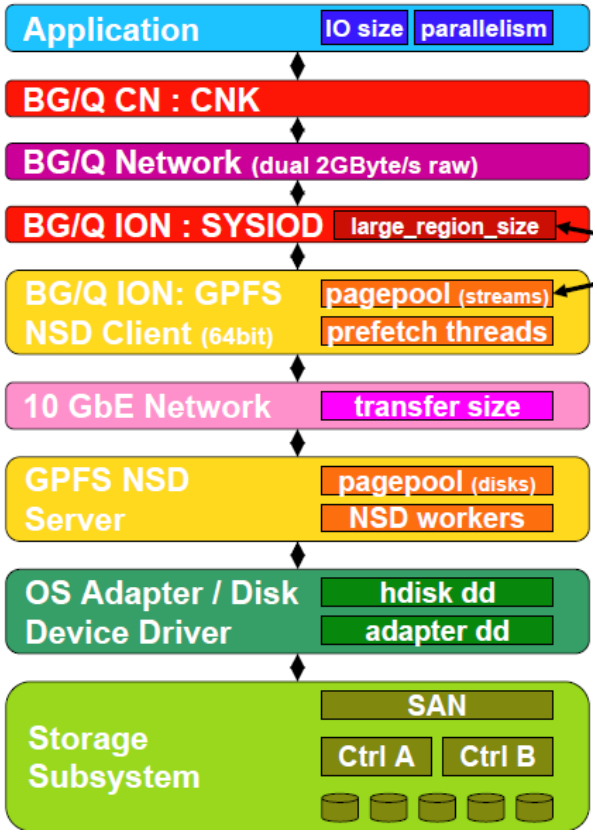
Blue Gene/Q: I/O Services

- Function shipping system calls to I/O-node
- Support NFS, GPFS, Lustre and PVFS2 filesystems
- Supports ratio of **8192:1** compute task to I/O-node
  - Only 1 I/O-Proxy per compute node
- Standard communications protocol
  - OFED verbs
  - Using Torus DMA hardware for performance



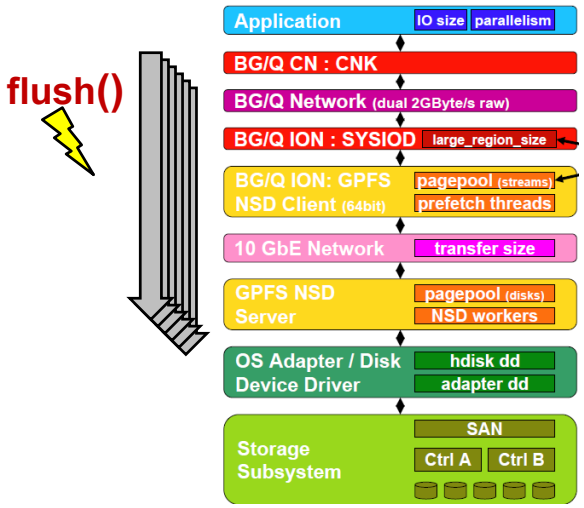
IBM General Parallel File System : Architecture and I/O Data Path on BG/Q



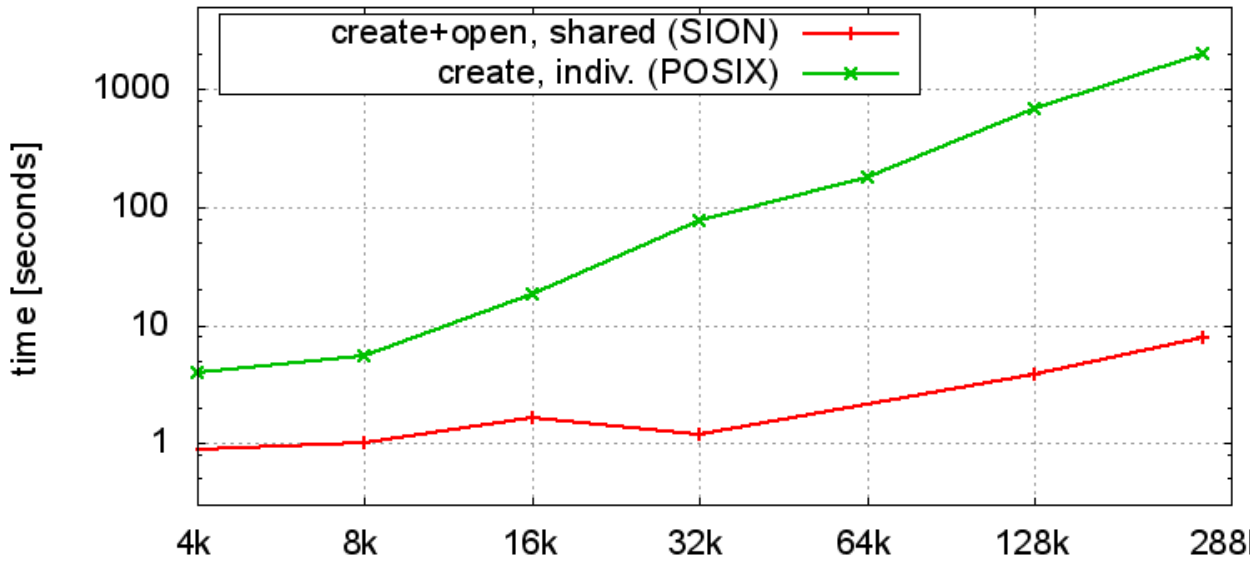


Pitfall 1: Frequent flushing on small blocks

- Modern file systems in HPC have large file system blocks
- A flush on a file handle forces the file system to perform all pending write operations
- If application writes in small data blocks the same file system block it has to be read and written multiple times
- Performance degradation due to the inability to combine several write calls



Pitfall 2: Parallel Creation of Individual Files

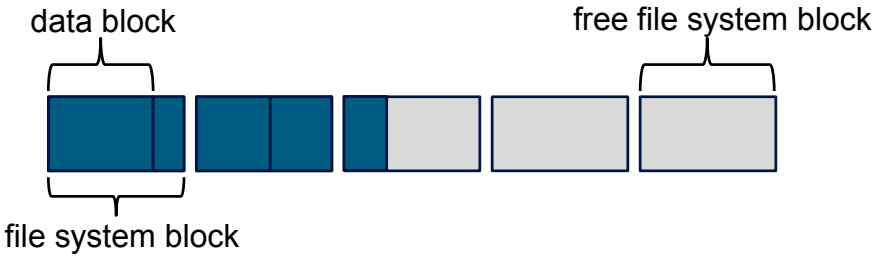


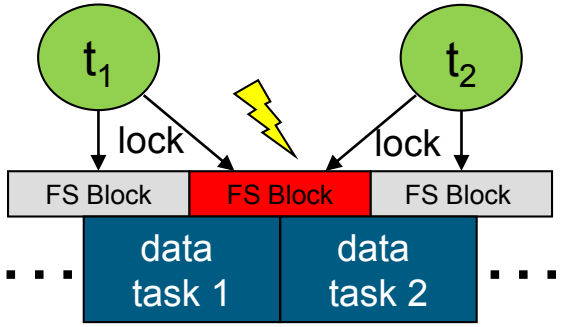
Jugene (BG/P) + GPFS: file create+open, one file per task versus one file per I/O-node

- Contention at node doing directory updates (directory meta-node)
- Pre-created files or own directory per task may help performance, but does not simplify file handling
- Complicates file management (e.g. archive) → **shared files are mandatory**

Pitfall 3: False sharing of file system blocks

- Parallel I/O to shared files (POSIX)

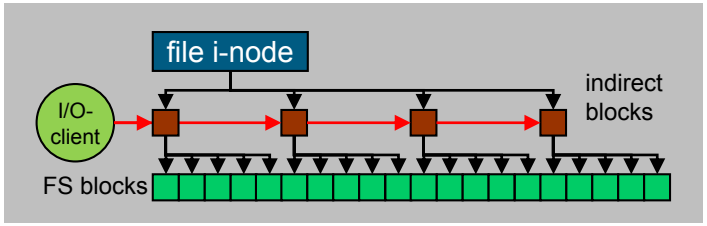




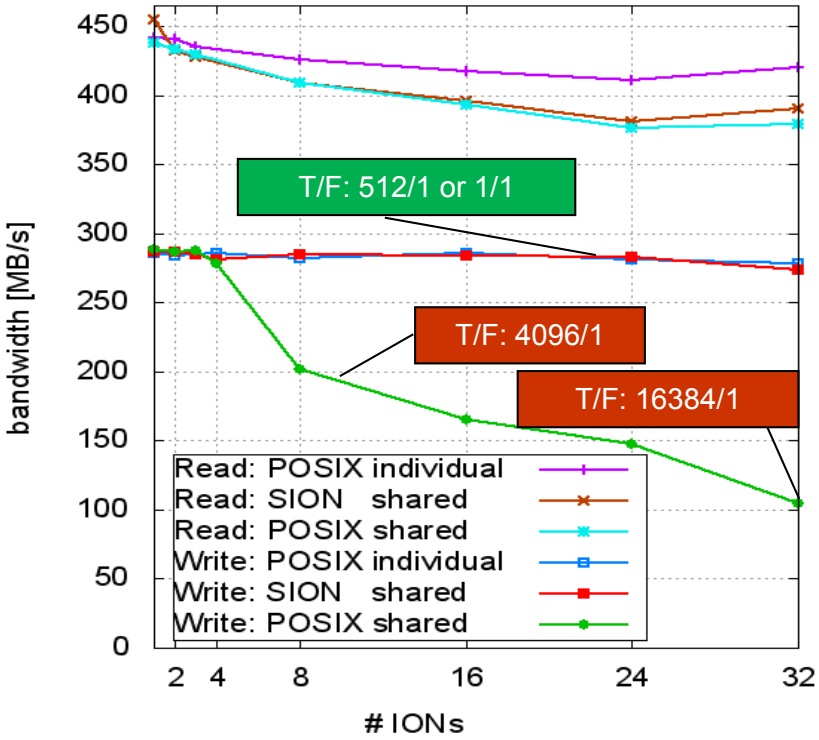
- Data blocks of individual processes do not fill up a complete file system block
- Several processes share a file system block
- Exclusive access (e.g. write) must be serialized
- The more processes have to synchronize the more waiting time will propagate

Pitfall 4: Number of Tasks per Shared File

- Meta-data wall on file level
  - File meta-data management
  - Locking



- Example Blue Gene/P
  - Jugene (72 racks)
  - I/O forwarding nodes (ION)
  - GPFS client on ION
  - Solution:
    - → tasks : files ratio ~ const
    - → SIONlib:
      one file per ION
      implicit task-to-file mapp



Pitfall 5: Portability

- Endianess (byte order) of binary data
- Example (32 bit):

2.712.847.316

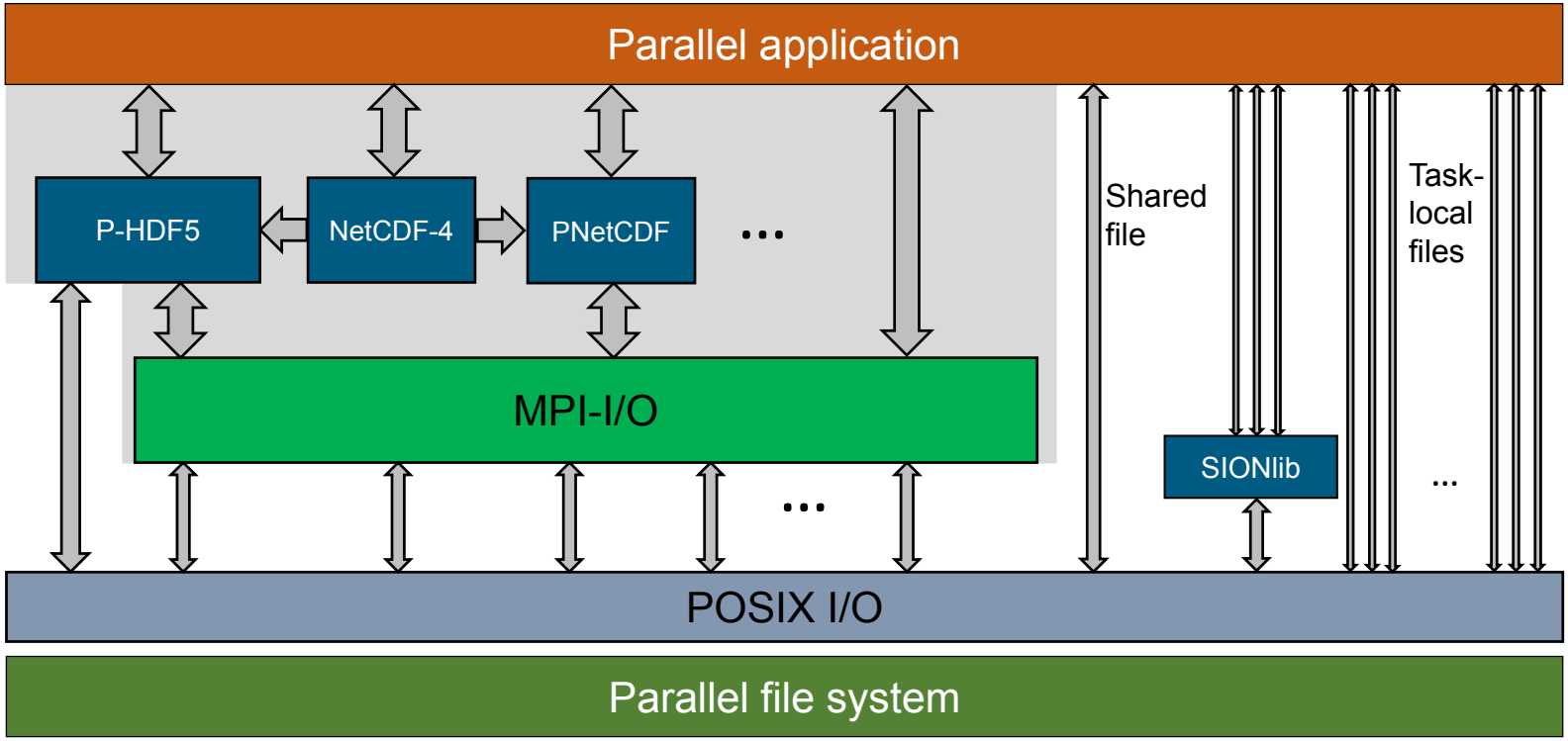
=

10100001 10110010 11000011 11010100

Address	Little Endian	Big Endian
1000	11010100	10100001
1001	11000011	10110010
1002	10110010	11000011
1003	10100001	11010100

- Conversion of files might be necessary and expensive
- Solution: Choosing a portable data format (HDF5, NetCDF)

The Parallel I/O Software Stack



How to choose an I/O strategy?

- Performance considerations
  - Amount of data
  - Frequency of reading/writing
  - Scalability
- Portability
  - Different HPC architectures
  - Data exchange with others
  - Long-term storage
- E.g. use two formats and converters:
  - Internal: Write/read data “as-is”
    → Restart/checkpoint files
  - External: Write/read data in non-decomposed format
    (portable, system-independent, self-describing)
    → Workflows, Pre-, Postprocessing, Data exchange, …

Darshan: Overview

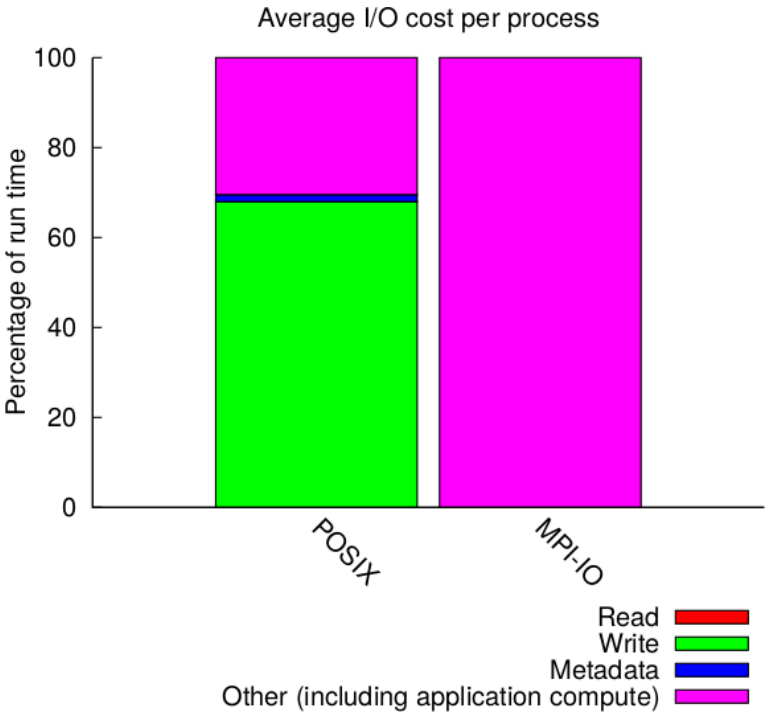
- Developed at ANL: http://www.mcs.anl.gov/darshan
- "HPC I/O Characterization Tool" instruments I/O
  - Uses modified versions of I/O libraries during linking
    - No code changes needed only recompilation with wrapped compiler
  - Helps analysing I/O patterns and identifying bottlenecks
  - Analyses parallel I/O with MPI-IO and standard POSIX I/O
- Ready to use version available on JUQUEEN

Darshan: Usage example on JUQUEEN

- Load module
  - module load darshan
- Recompile
  - make MPICC=mpicc.darshan
- Tell runjob where to save the output (in submit script)
  - runjob ... --envs \
    DARSHAN_LOG_PATH=$HOME/darshanlogs …
- Analyse output
  - darshan-job-summary.pl mylog.darshan.gz
  - evince mylog.pdf

Darshan: Interpret the summary

- Average and statistical information on I/O patterns
  - Relative time for I/O
  - Most common access sizes
- Additional metrics
  - File count
  - I/O size histogram
  - Timeline for read / write per task
  - …

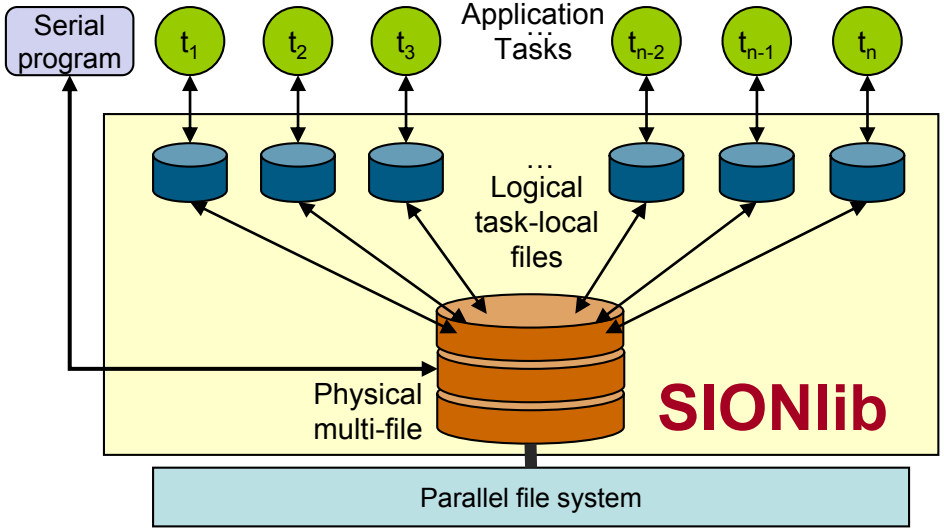


Most Common Access Sizes

access size	count
4194304	256

SIONlib: Overview

- Shared file I/O with automatic file system block alignment
  - One single or few large files (e.g. one per ION)
    - Only open and close calls are collective
  - Support for file coalescing
    - For data sizes << file system block size
- http://www.fz-juelich.de/jsc/sionlib



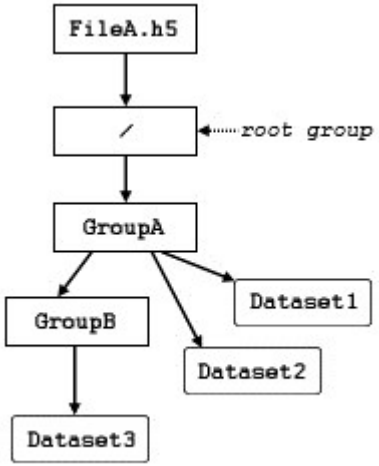

```
/* fopen() → */
sid=sion_paropen_mpi( filename , “bw“,
                      &numfiles, &chunksize,
                      gcom, &lcom, &fileptr, ...);

/* fwrite(bindata,1,nbytes, fileptr) → */
sion_fwrite(bindata,1,nbytes, sid);

/* fclose() → */
sion_parclose_mpi(sid)
```

Parallel HDF5: Overview

- Self-describing file format
  - Hierarchical, filesystem-like data format
  - Support of additional metadata for datasets
- Portable
  - Builds on top of standard MPI-I/O or POSIX-I/O
  - Move between system architectures
    - Automatic conversion of data representation
  - Move between parallel/serial applications
    - e.g. 4096 MPI processes → 65.536 MPI processes
    - e.g. simulation → post-processing
  - Complex data selections possible for read or write
    - e.g. read only sub-array of dataset with stride



slide provided by Jens Henrik Göbbert

Parallel HDF5: I/O Hints

- Align datasets to file system block size

```
H5Pset_alignment(...);
```

- Use hyperslabs

```
H5Sselect_hyperslab(...);
```

- Chunk datasets

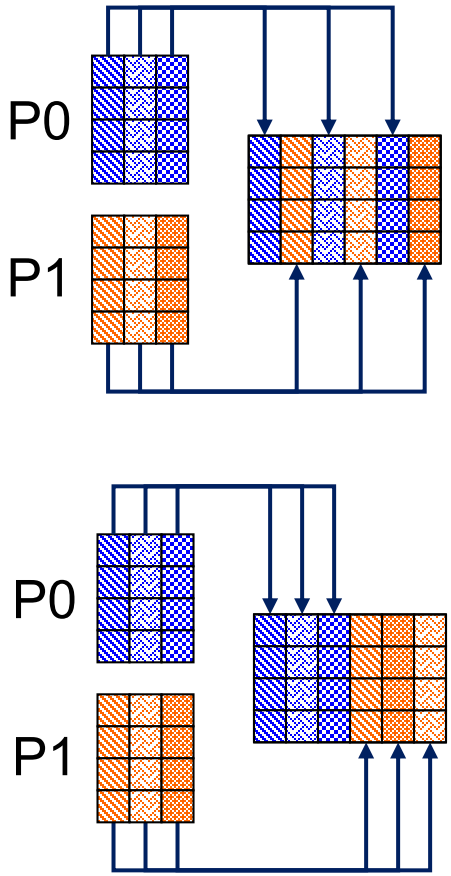
```
H5Pset_cache(...);
H5Pset_chunk_cache(...);
```

- Increase transfer buffer

```
H5Pset_buffer(...);
```

- Improve metadata handling

```
H5Pset_istore_k(...);
H5Pset_meta_block_size(…);
```



slide provided by Jens Henrik Göbbert

I/O Hints

- Reduce locking for MPI-IO
  - export BGLOCKLESSMPIO_F_TYPE="0x47504653“
- ROMIO hints
  - echo " IBM_largeblock_io true" > romio.hints
  - echo " cb_buffer_size 33554432" >> romio.hints
  - export ROMIO_HINTS=romio.hints
- Note: don’t forget to add exports to runjob, via “--exp-env X”
- MPIX_Calls: splitting communicators per I/O-bridge

```
FORTRAN: MPIX_PSET_SAME_COMM_CREATE(INTEGER pset_comm_same,
                                    INTEGER ierr)
C: #include <mpix.h>
   int MPIX_Pset_same_comm_create( MPI_Comm *pset_comm_same )
```

sid=**sion_paropen_mpi**(filename , “bw“, &numfiles, &chunksize, gcom, &lcom, ...);